Multi-scale Molecular Dynamics and Parallelization for Blue Gene/Q

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Simulating the molecular dynamics of condensed phase biological molecules is a formidable computational challenge, often involving thousands to millions of atoms, many degrees of freedom, and relatively long time scales. Further, simulation of inherently quantum mechanical phenomena, such as proton transfer, can add another layer of complexity into the molecular dynamics. High performance computing offers a means to carry out such simulations, yet it too can be a challenge of its own, requiring careful attention to details in parallel algorithms and coding paradigms.

In this presentation, we will discuss our preparations to dispatch large-scale multi-scale molecular dynamics simulations on Argonne's new state-of-the-art Blue Gene/Q supercomputer, Mira, as part of the Early Science Program at the Argonne Leadership Computing Facility. Specifically, we will focus on the Multi-State Empirical Valence Bond method for the simulation of proton transfer in biological systems, such as charge transport through membrane proteins. Our efforts to implement improved parallelization under a hybrid OpenMP/Message Passing Interface paradigm will be shown. In addition, we will discuss multi-replica ensemble simulations and their propensity to scale efficiently over several racks of Mira.